SCATTERING OF ELECTRON BY THOMAS-FERMI POTENTIAL

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ABSTRACT. In this paper the elastic scattering cross-section of electrons by the Thomas-Fermi potential as represented by the analytical forms due to Gombas and Tietz has been calculated by the Born approximation method. Our results are in fair agreement with those calculated with the exact numerical form of Thomas-Fermi potential. Further comparison shows that the Gombas-Tietz form is as good as those of Rozental and Buchdahl.

INTRODUCTION

The scattering of electron by a heavy atom is a many body problem, the electron to be scattered is influenced by the positively charged nucleus and the negatively charged electrons surrounding the nucleus. It is difficult to calculate accurately the electrical potential due to such an atom. Of the two available methods, the self-consistent field method of Hartree and Fock is more accurate than the statistical one of Thomas and Fermi. The difficulty of calculation by Hartree's method increases with the complexity of the atom, whereas the more complex the atom is the more valid is the calculation for the Thomas-Fermi potential, because the electrons of the complex atom are treated as a statistical ensemble. The form of the Thomas-Fermi potential is taken to be

$$V(r) = -\frac{Ze^2}{r}\phi(x)$$

where ϕ is the Thomas-Fermi function for the free neutral atom and is the solution of

$$\frac{\partial^2\phi}{\partial x^2} = \frac{\phi^{3/2}}{x^{\frac{1}{2}}}$$

where $x = r/\mu$; $\mu = \frac{0.88534}{Z^{1/3}}\, a_0$, a_0 being the first Bohr radius and Z is the atomic number. The above equation does not admit of an exact solution which is available only in the form of a numerical table; however, various approximations in analytical forms have been suggested by several authors like Sommerfeld (1932), Rozental (1935), Gombas (1949), March (1950), Kerner (1951), Tietz

(1955, 1956), Brinkman (1954), Umeda (1955), Buchdahl (1956) and Latter (1955). It is not possible to calculate analytically the scattering cross section with the forms of Sommerfeld, March, Umeda and Latter. The form of Kerner is not quite suitable. Majewasky and Tietz (1957) have calculated scattering cross section in the Born approximation with the forms of Brinkman, Buchdahl and Rozental. The form of Gombas (1949) is valid only in a region near the nucleus and that of Tietz (1954) holds good outside this region. We propose to calculate the scattering cross section with the Gombas-Tietz form. We are led to this choice of the potential, because Tsang (1959) taking the form of Gombas has got good agreement of binding energies of electrons with those obtained by using the Thomas-Fermi potential and by Hartree's method. In this paper we have calculated by the Born approximation method the elastic scattering cross section of electrons by a central potential which is of the form of Gombas between the range $0 \leqslant x \leqslant 1$ and of Tietz for $x \geqslant 1$. We have compared our findings obtained by such a potential with the results of Mott and Massey (1949) obtained with Thomas-Fermi potential and that of Tietz and Majewasky (1957) calculated with the potentials of Rozental (1935) and Buchdahl (1956).

For electrons having 50 KeV energy scattered by Krypton ($Z=36$) the differential cross section decreases with increasing angle upto 70° ; thereafter it fluctuates with two maxima at 80° and 110°. Unfortunately there is no experimental data to compare with our theoretical findings.

CALCULATION

The amplitude of scattering by a central potential $V(r)$, according to the Born approximation, is given by

$$f(\theta) = -\frac{8\pi^2 m}{h^2} \int_0^\infty \frac{\sin kr}{kr} V(r) r^2 dr \qquad \ldots (1)$$

where θ is the scattering angle,

$$K = k\ |n_0 - n| = \frac{4\pi \sin \theta/2}{\lambda} \ ; \ \lambda = \frac{2\pi}{k} = \frac{h}{mv}$$

n_0 being the unit vector along the Z-axis, n is a unit vector along the direction of r.

In the case of scattering of electrons by an atom we choose the potential as

$$V(r) = V_G \quad \text{valid for } 0 \leqslant x \leqslant 1 \qquad \ldots (2)$$

$$= V_T \quad \text{valid for } x \geqslant 1$$

where V_G has the form as given by Gombas,

$$V_G = -\frac{Ze^2}{x\mu}\{0.878-0.546x+0.415(x-0.5)^2\}$$

where $x = \frac{r}{\mu}$; $\mu = \frac{0.88534}{Z^{1/3}}\, a_0$, and a_0 being the first Bohr radius for hydrogen and Z is the atomic number, and the form of V_T is due to Tietz,

$$V_T = -\frac{Ze^2}{x\mu}\left\{\frac{a^2}{(x+a)^2}\right\}$$

where $a = 1.86$, the values of x and μ are the same as in V_G. Substituting the form of (2) in Eq. (1), we get

$$f(\theta) = -\frac{8\pi^2 m\mu^3}{h^2 p}\left\{\int_0^1 \sin px\, V_G x dx + \int_1^\infty \sin px\, V_T x dx\right.$$

where

$$p = 2\mu k \sin\theta/2 = K\mu$$

$$K = 2k \sin\theta/2.$$

$$\therefore \quad \frac{f(\theta)}{Z^{1/3}} = \frac{83.07\times 10^{-10}}{p}\left[\sin p\left(-\frac{0.131}{p^2}\right) + \cos p\left(\frac{0.830}{p^3} - \frac{0.435}{p}\right)\right.$$

$$+ \frac{0.981}{p} - \frac{0.830}{p^3} + a^2\left\{\frac{\sin p}{1+a} - p\left(\cos pa\, Ci\{p(1+a)\} + \sin pa\, Si\{p(1+a)\}\right.\right.$$

$$\left.\left.\left. - \sin pa\, \frac{\pi}{2}\right)\right\}\right]$$

where $Si(x) = \int \frac{\sin t}{t}\, dt$; $Ci(x) = -\int_x \frac{\cos t}{t}\, dt$

For the sake of comparison we give also the results of Tietz and Majewasky (1957) who have calculated the same with the potential forms of Rozental and Buchdahl.

The Rozental form is as follows :

$$\phi(x) = \sum_{i=1}^{3} C_i\, e^{-a_i x}$$

where C_i and a_i are constants and their values are $c_1 = 0.255$, $c_2 = 0.581$, $c_3 = 0.164$, $a_1 = 0.246$, $a_2 = 0.947$, $a_3 = 4.356$.

The Buchdahl form is as follows :

$$\phi(x) = [(1+Ax)(1+Bx)(1+Cx)]^{-1}$$

where $A = 0.9288$, $B = 0.1536$, $C = 0.05727$.

TABLE I

Comparison of our results for $|f(\theta)|^2$ with the numerical results of Mott and Massey and results of Rozental and Buchdahl

	$\|f(\theta)\|^2 Z^{-2/3}$ in units of 10^{-18}cm^2			
$p=2\mu K \sin\theta/2$	Mott & Massey	Rozental	Buchdahl	Present author
0.1	1460	1525	1257	1296
0.2	678	654	690	642
1.0	18.7	17.1	21.2	20.79
2.0	2.52	2.49	2.45	2.74
5.0	0.089	0.096	0.091	0.094
6.0	0.047	0.048	0.046	0.051
8.0	0.016	0.016	0.017	0.016
10.0	0.0064	0.0063	0.0065	0.0057

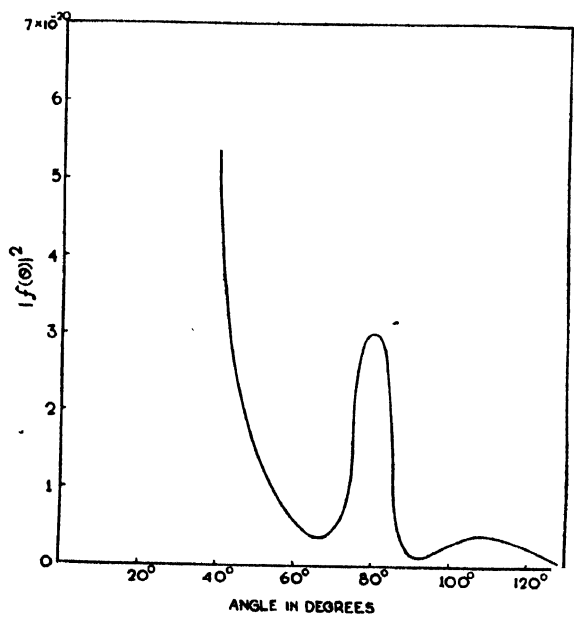

Fig. 1. Angular distribution of electrons at 40 KeV scattered by krypton (z=36)

DISCUSSION

From the table of comparison it appears that our result of differential scattering cross section calculated with the Gombas-Tietz form agrees pretty well with the results of Mott and Massey. Our results are as good as those calculated with the forms of Rozental and Buchdahl.

From the calculation it is found that when p is large the contribution to the scattering from the Gombas potential is much larger than that from the Tietz potential whereas when p is small the reverse is the case. This finding is in conformity with the physical picture; the larger the value of p is, greater is the number of particles coming under the influence of Gombas part of the potential.

For 50 KeV electrons scattered by Krypton ($Z = 36$) the differential cross section decreases with increasing angle till 70°, after which there are small rise and fall of the values giving two maxima which are analogous to diffraction phenomenon.

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7

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